

**Calliviminones C-H: Six New Hetero- and Carbon-Diels-Alder
Adducts with Unusual Skeletons from the Fruits of *Callistemon
viminalis***

Lin Wu, Jun Luo, Xiao-bing Wang, Rui-jun Li, Ya-long Zhang and Ling-Yi Kong*

*State Key Laboratory of Natural Medicines, Department of Natural Medicinal Chemistry, China Pharmaceutical
University, 24 Tong Jia Xiang, Nanjing 210009, People's Republic of China*

The list of supplementary content

Figure S1.1 ^1H NMR spectrum of compound 1 in CDCl_3	4
Figure S1.2 ^{13}C NMR spectrum of compound 1 in CDCl_3	4
Figure S1.3 HSQC spectrum of compound 1 in CDCl_3	5
Figure S1.4 HMBC spectrum of compound 1 in CDCl_3	5
Figure S1.5 ROESY spectrum of compound 1 in CDCl_3	6
Figure S1.6 HRESIMS spectrum of compound 1	6
Figure S2.1 ^1H NMR spectrum of compound 2 in CDCl_3	7
Figure S2.2 ^{13}C NMR spectrum of compound 2 in CDCl_3	7
Figure S2.3 HSQC spectrum of compound 2 in CDCl_3	8
Figure S2.4 HMBC spectrum of compound 2 in CDCl_3	8
Figure S2.5 ROESY spectrum of compound 2 in CDCl_3	9
Figure S2.6 HRESIMS spectrum of compound 2	9
Figure S3.1 ^1H NMR spectrum of compound 3 in CDCl_3	10
Figure S3.2 ^{13}C NMR spectrum of compound 3 in CDCl_3	10
Figure S3.3 HSQC spectrum of compound 3 in CDCl_3	11
Figure S3.4 HMBC spectrum of compound 3 in CDCl_3	11
Figure S3.5 ROESY spectrum of compound 3 in CDCl_3	12
Figure S3.6 HRESIMS spectrum of compound 3	12
Figure S4.1 ^1H NMR spectrum of compound 4 in CDCl_3	13
Figure S4.2 ^{13}C NMR spectrum of compound 4 in CDCl_3	13
Figure S4.3 HSQC spectrum of compound 4 in CDCl_3	14

Figure S4.4 HMBC spectrum of compound 4 in CDCl ₃	14
Figure S4.5 ROESY spectrum of compound 4 in CDCl ₃	15
Figure S4.6 HRESIMS spectrum of compound 4	15
Figure S5.1 ¹ H NMR spectrum of compound 5 in CDCl ₃	16
Figure S5.2 ¹³ C NMR spectrum of compound 5 in CDCl ₃	16
Figure S5.3 HSQC spectrum of compound 5 in CDCl ₃	17
Figure S5.4 HMBC spectrum of compound 5 in CDCl ₃	17
Figure S5.5 ROESY spectrum of compound 5 in CDCl ₃	18
Figure S5.6 HRESIMS spectrum of compound 5	18
Figure S5.7 CD spectrum of compound 5	19
Figure S6.1 ¹ H NMR spectrum of compound 6 in CDCl ₃	19
Figure S6.2 ¹³ C NMR spectrum of compound 6 in CDCl ₃	20
Figure S6.3 HSQC spectrum of compound 6 in CDCl ₃	20
Figure S6.4 HMBC spectrum of compound 6 in CDCl ₃	21
Figure S6.5 ROESY spectrum of compound 6 in CDCl ₃	21
Figure S6.6 HRESIMS spectrum of compound 6	22
Figure S6.7 CD spectrum of compound 6	22

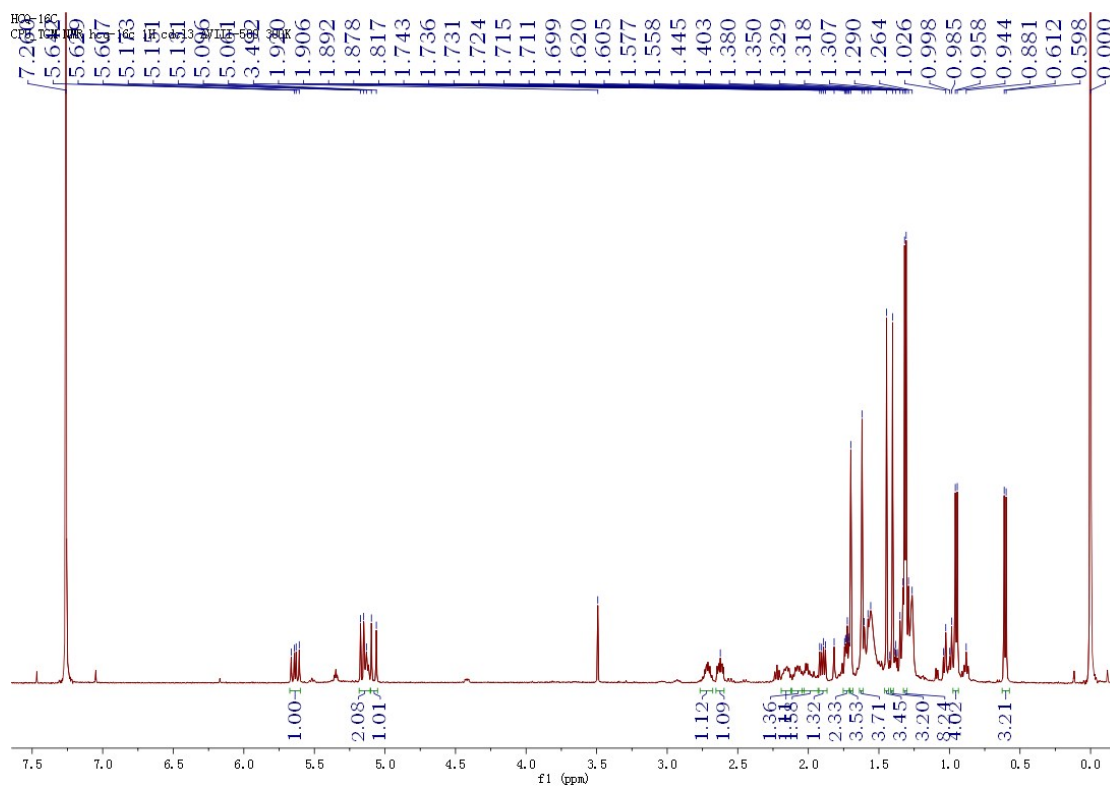


Figure S1.1 ^1H NMR spectrum of compound **1** in CDCl_3

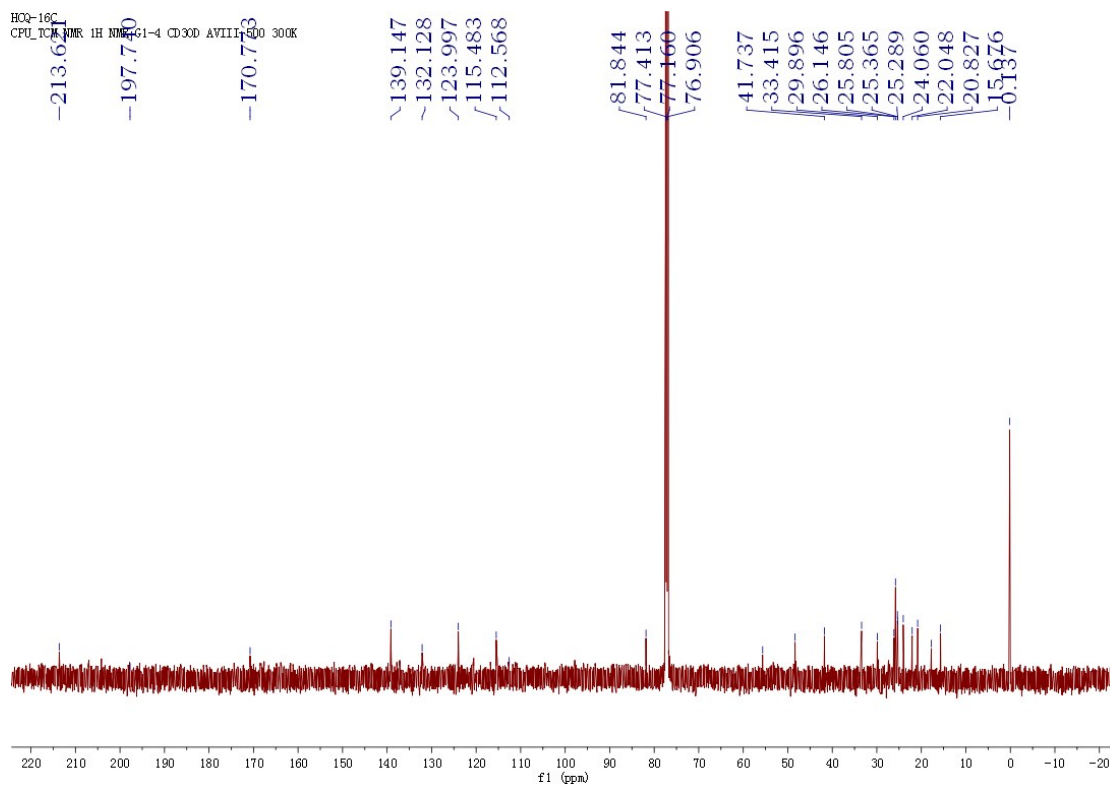


Figure S1.2 ^{13}C NMR spectrum of compound **1** in CDCl_3

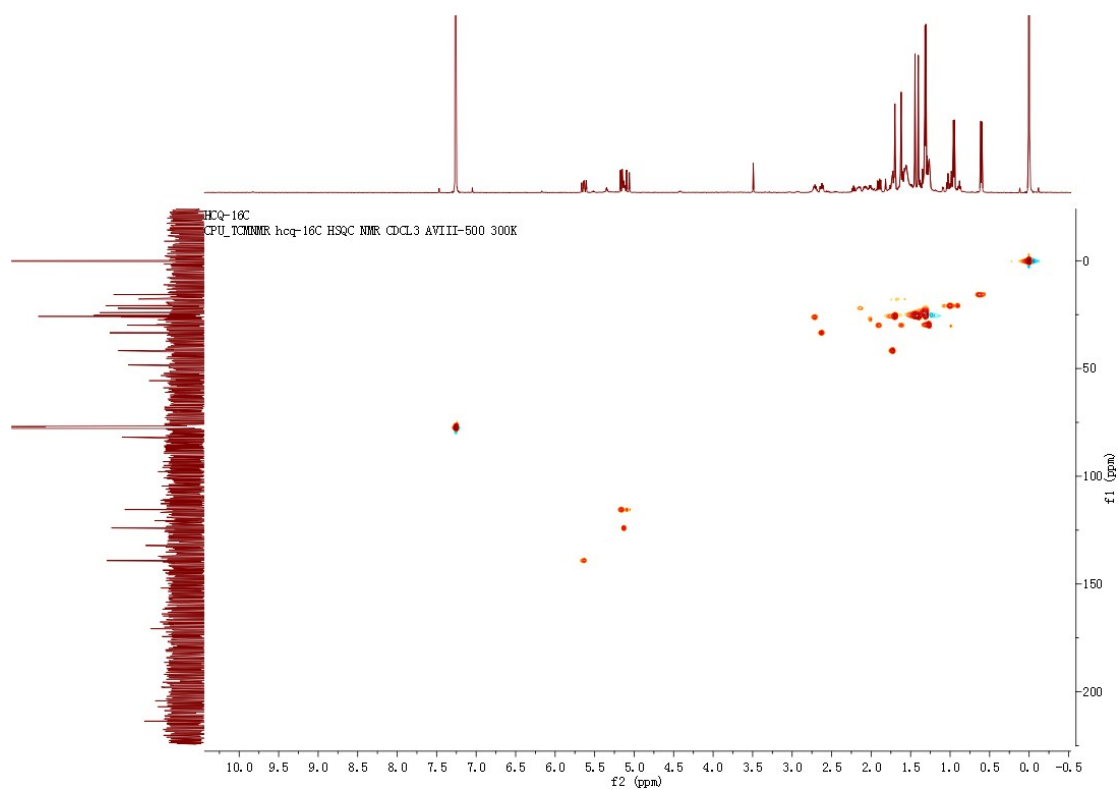


Figure S1.3 HSQC spectrum of compound **1** in CDCl₃

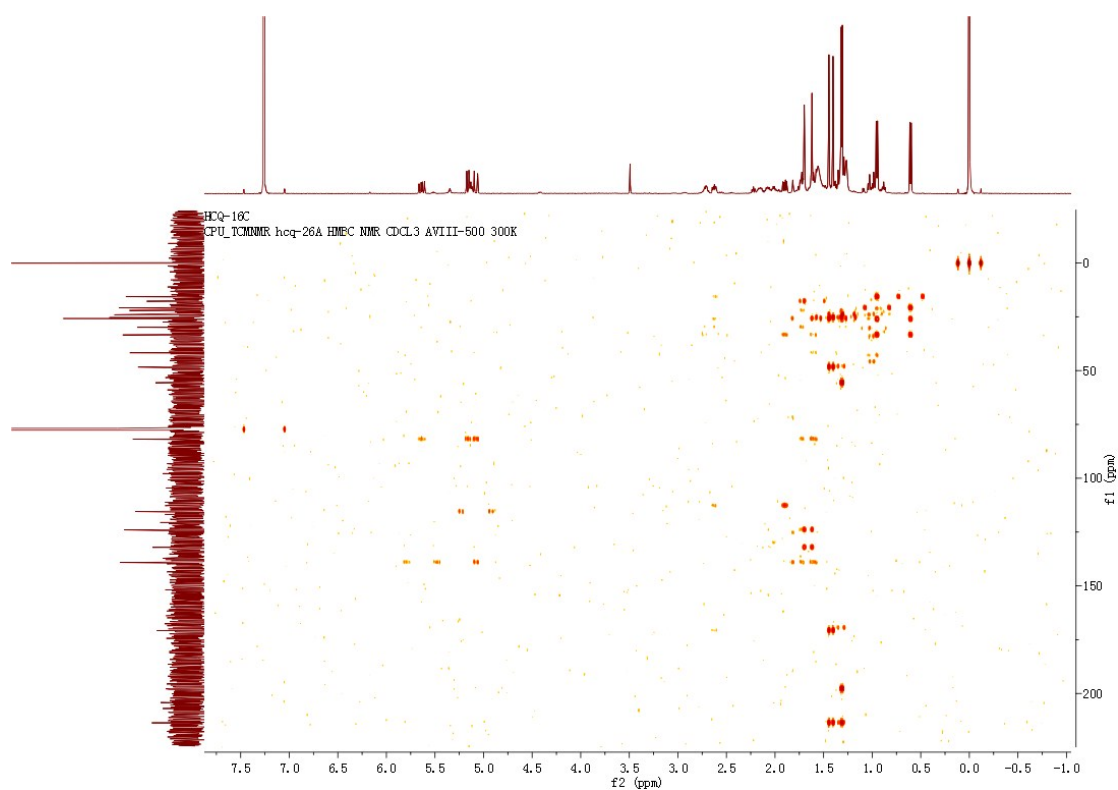


Figure S1.4 HMBC spectrum of compound **1** in CDCl₃

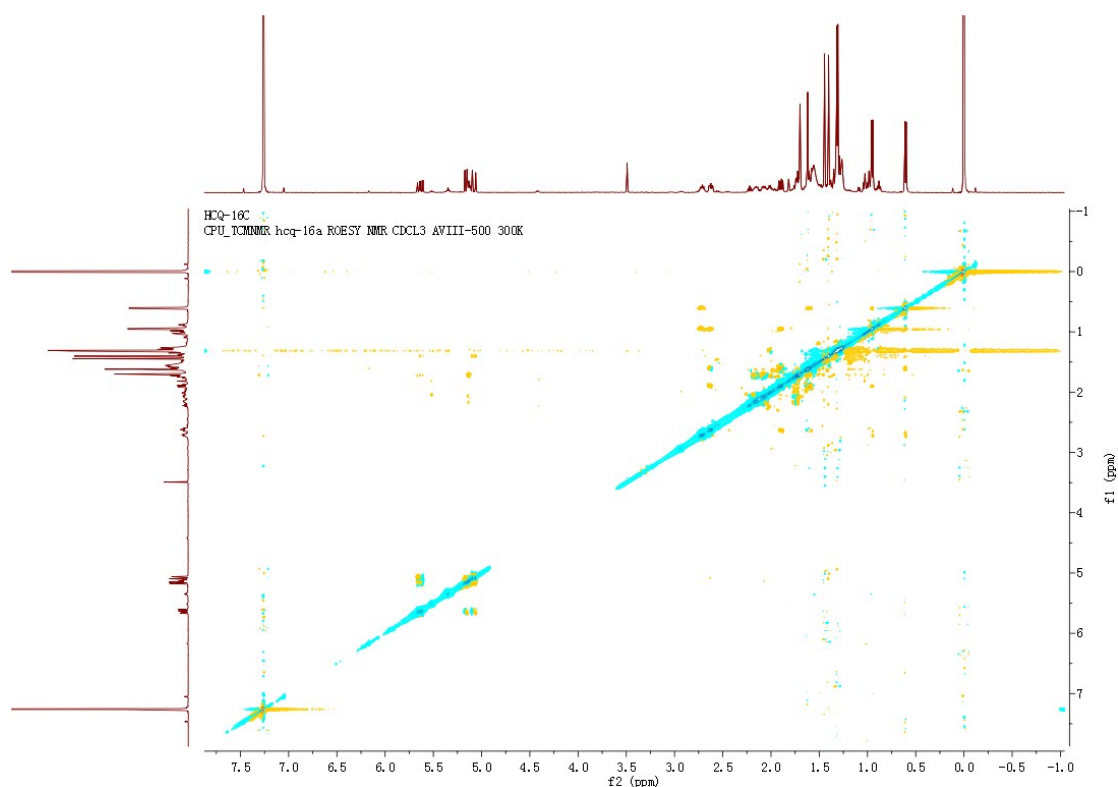
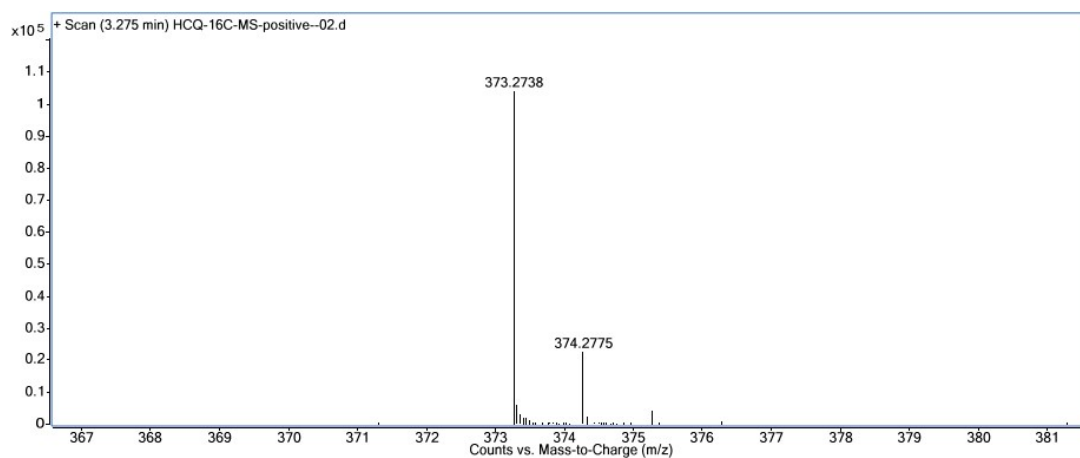


Figure S1.5 ROESY spectrum of compound **1** in CDCl₃



Elemental Composition Calculator

Target m/z:	373.2738	Result type:	Positive ions	Species:	[M+H] ⁺
Elements:	C (0-80); H (0-120); O (0-30); N(0-10); Na (0-5)				
Ion Formula	Calculated m/z		PPM Error		
C ₂₄ H ₃₇ O ₃	373.2737		-0.21		

Figure S1.6 HRESIMS spectrum of compound **1**

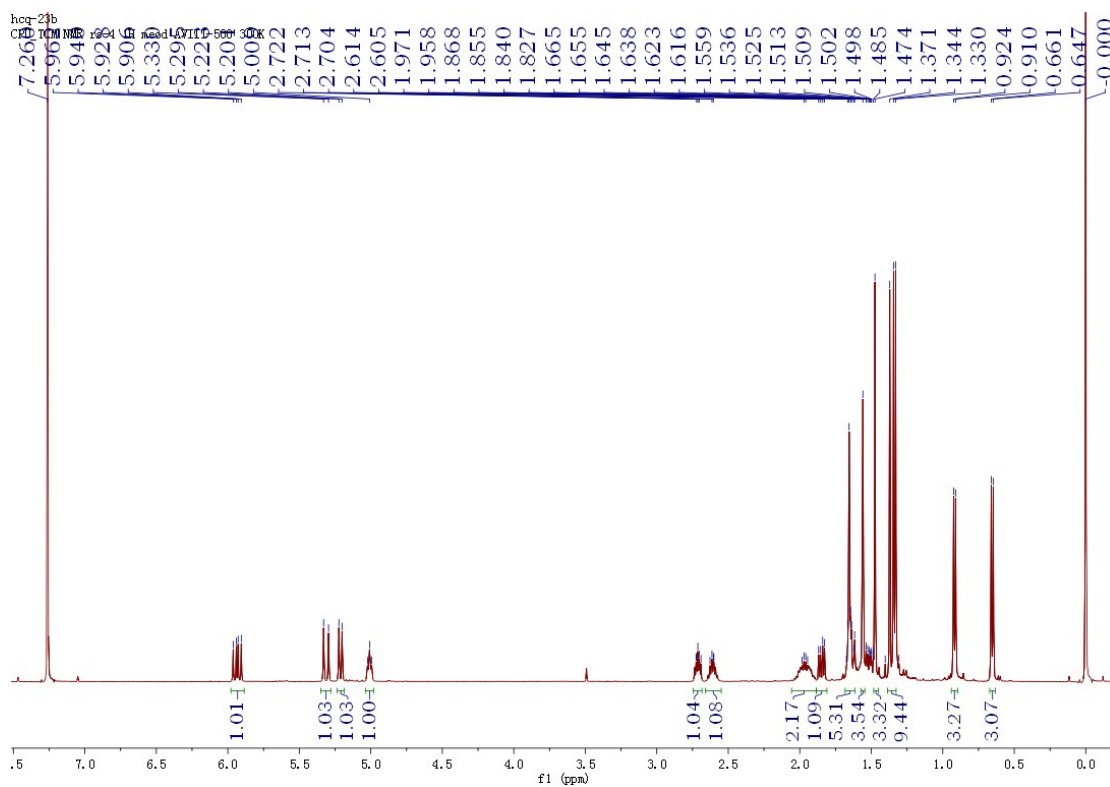


Figure S2.1 ^1H NMR spectrum of compound **2** in CDCl_3

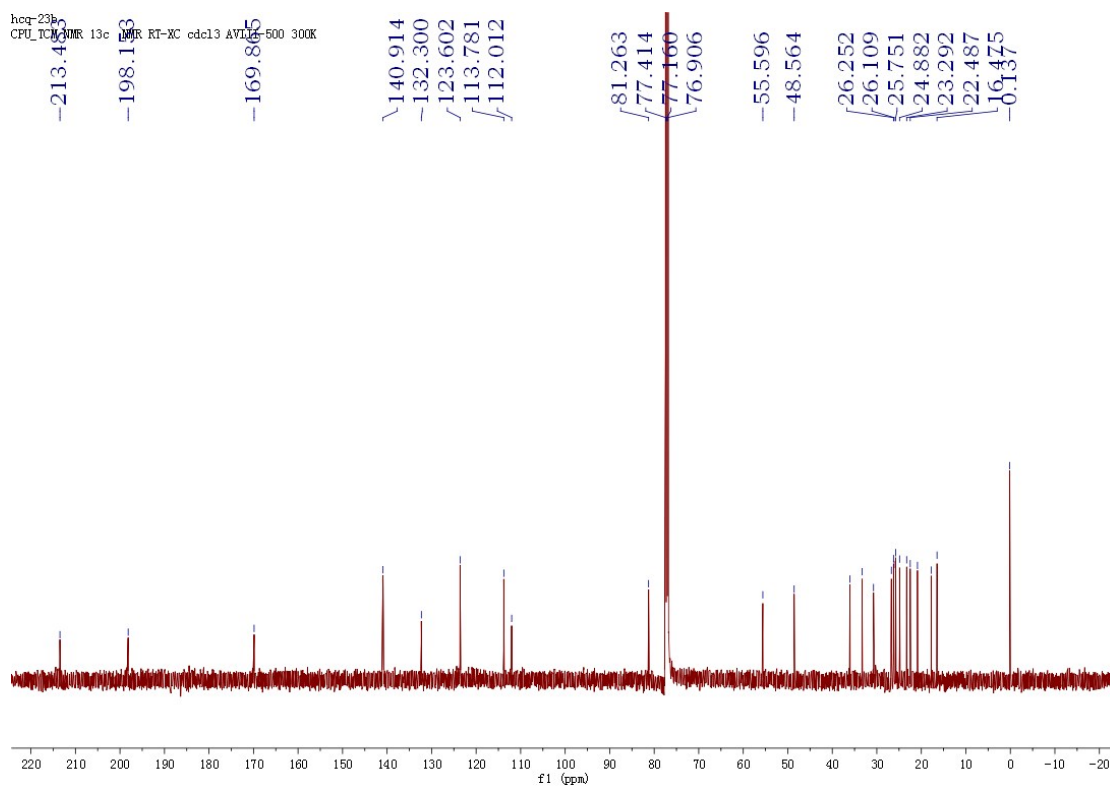


Figure S2.2 ^{13}C NMR spectrum of compound **2** in CDCl_3

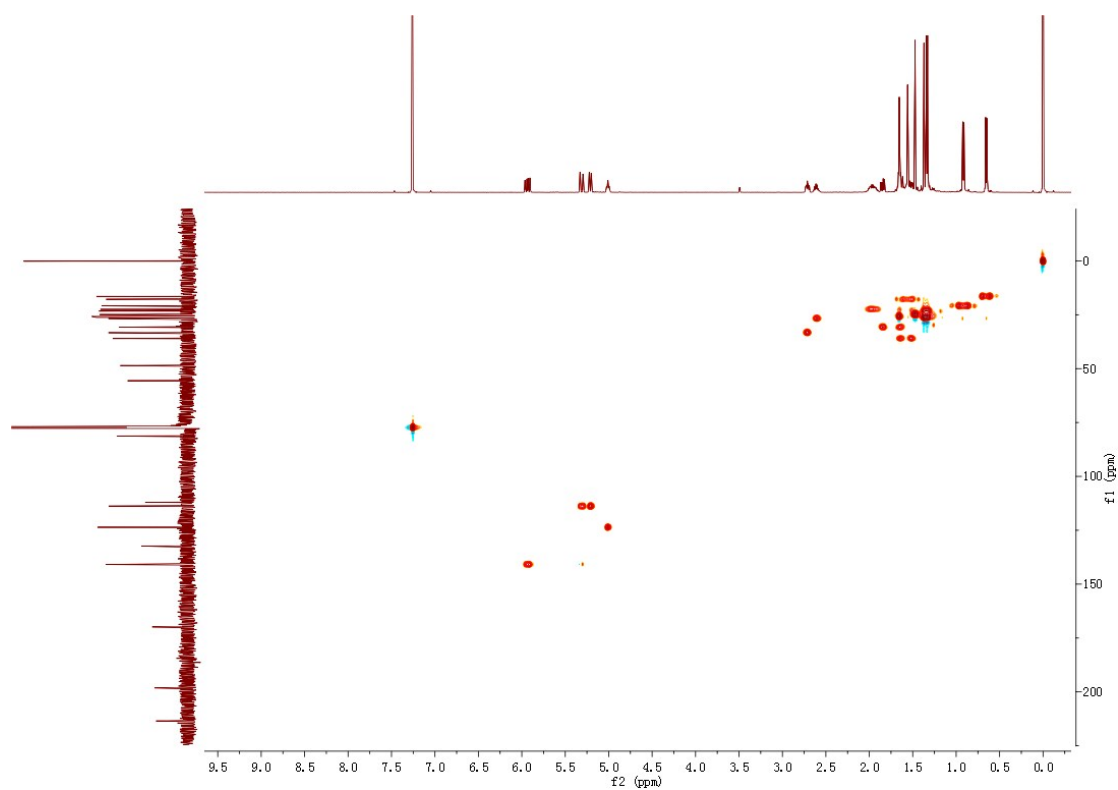


Figure S2.3 HSQC spectrum of compound **2** in CDCl_3

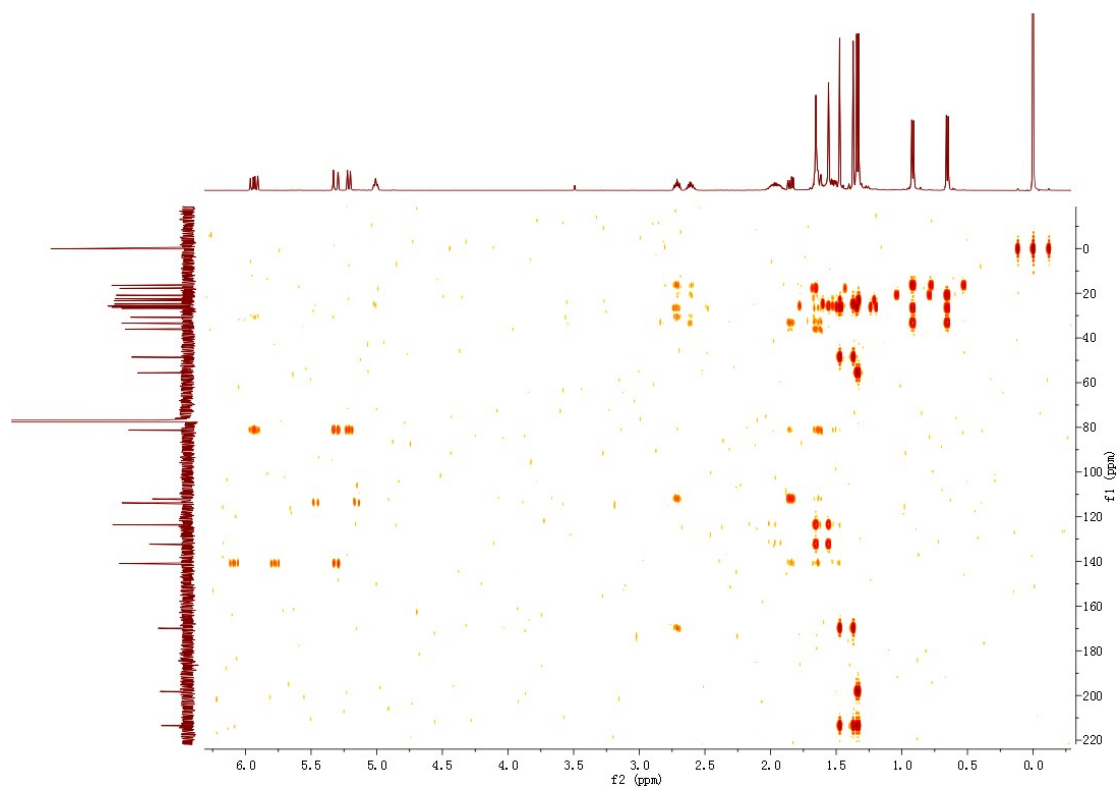


Figure S2.4 HMBC spectrum of compound **2** in CDCl_3

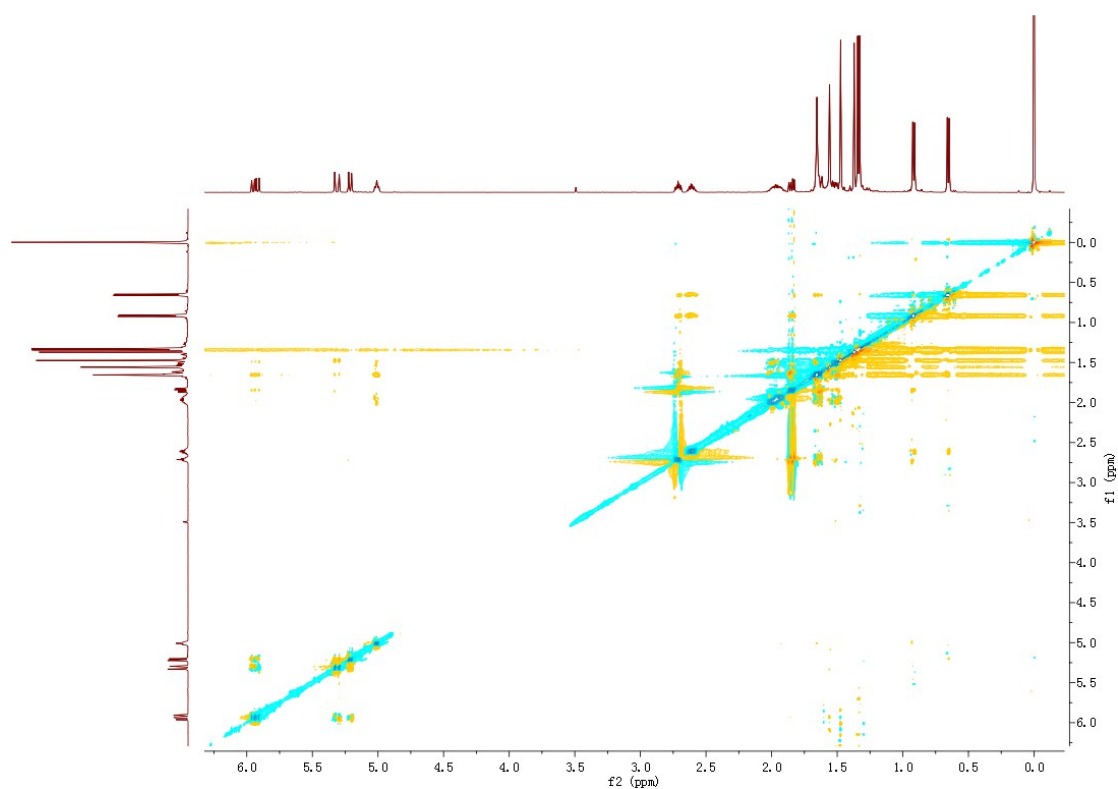
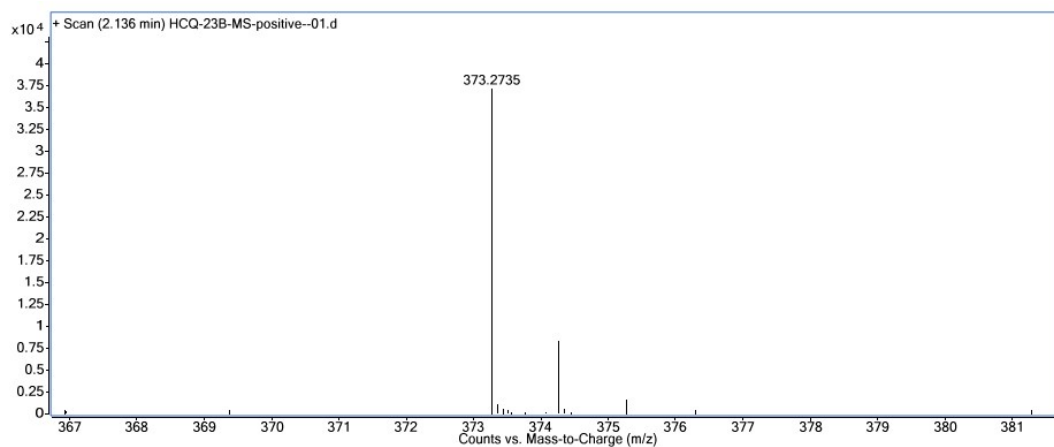


Figure S2.5 ROESY spectrum of compound **2** in CDCl₃



Elemental Composition Calculator

Target m/z:	373.2735	Result type:	Positive ions	Species:	[M+H] ⁺
Elements:	C (0-80); H (0-120); O (0-30); N(0-10); Na (0-5)				
Ion Formula	Calculated m/z		PPM Error		
C ₂₄ H ₃₇ O ₃	373.2737		0.61		

Figure S2.6 HRESIMS spectrum of compound **2**

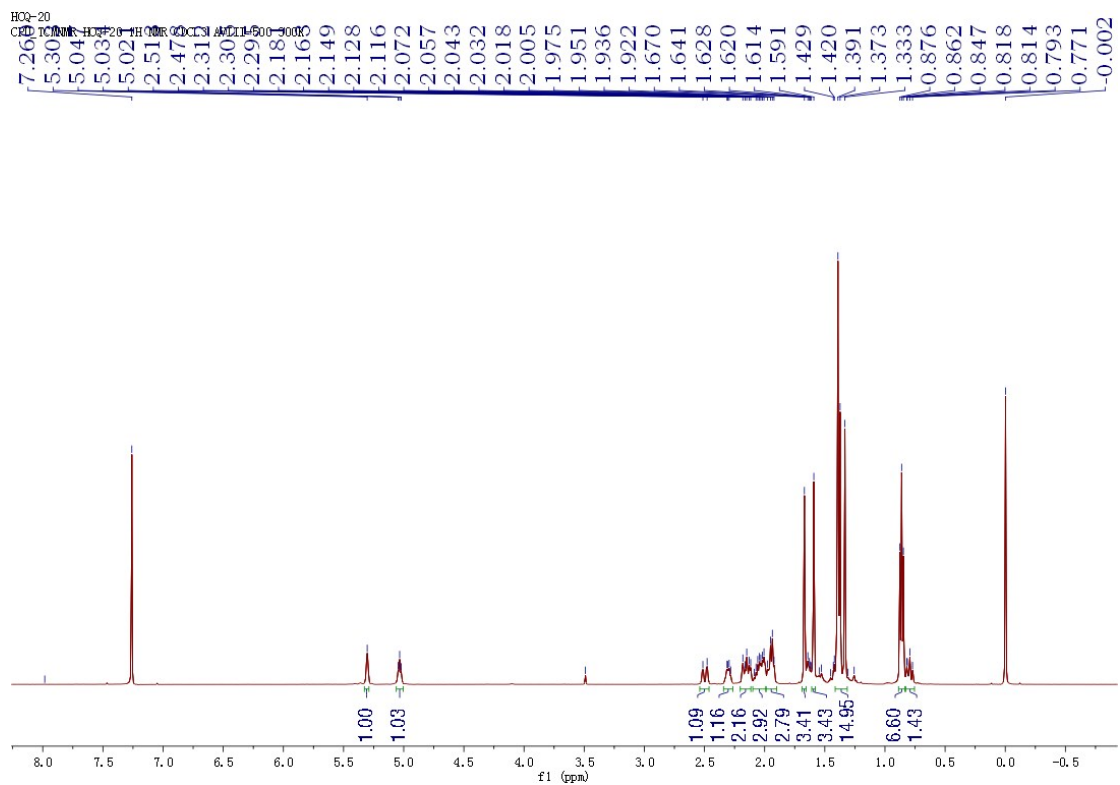


Figure S3.1 ¹H NMR spectrum of compound **3** in CDCl₃

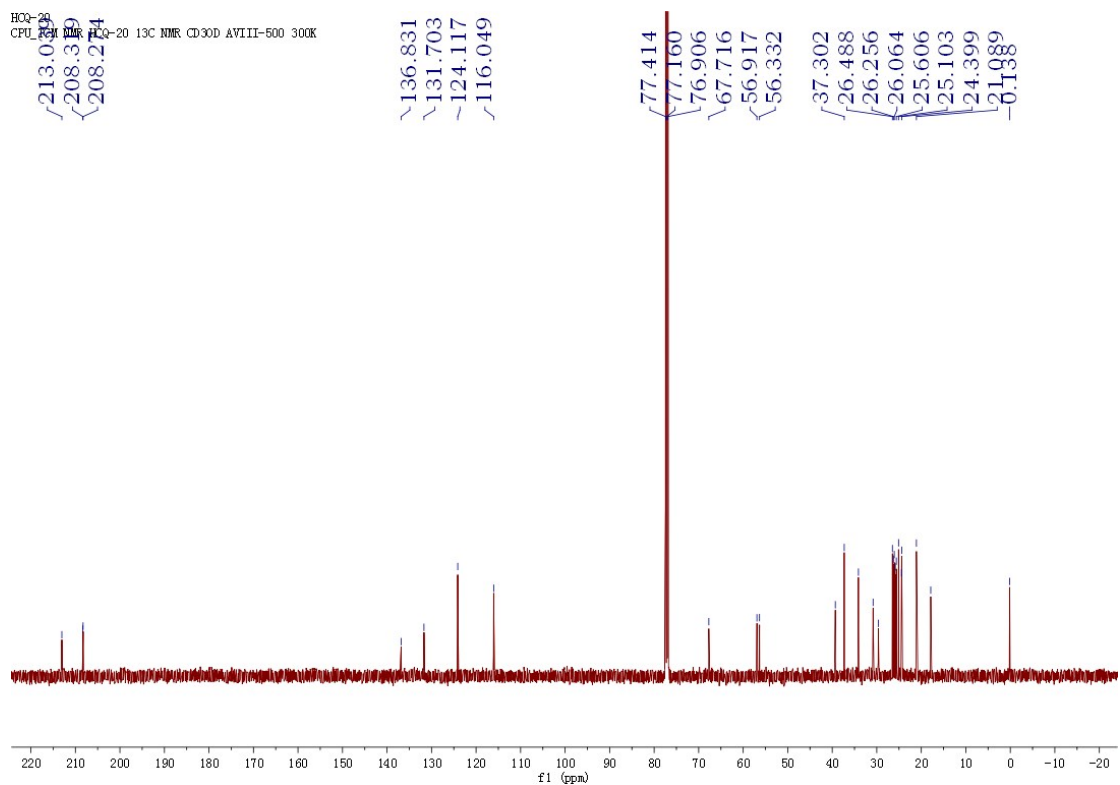


Figure S3.2 ¹³C NMR spectrum of compound **3** in CDCl₃

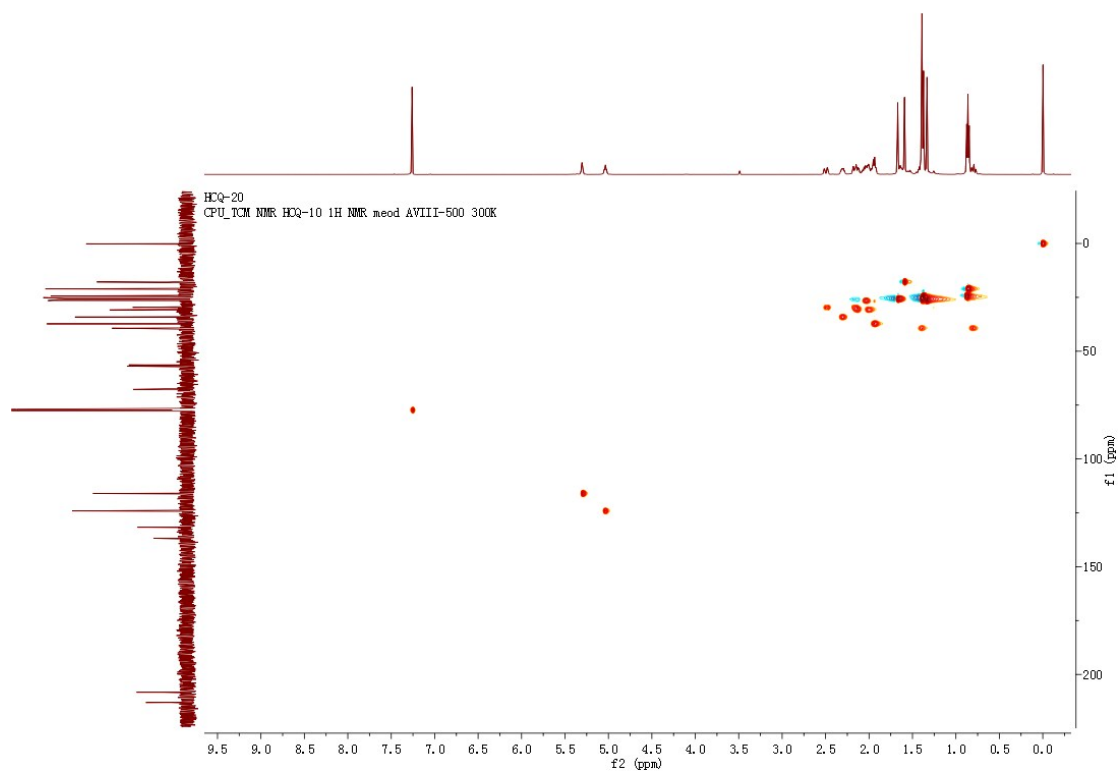


Figure S3.3 HSQC spectrum of compound **3** in CDCl_3

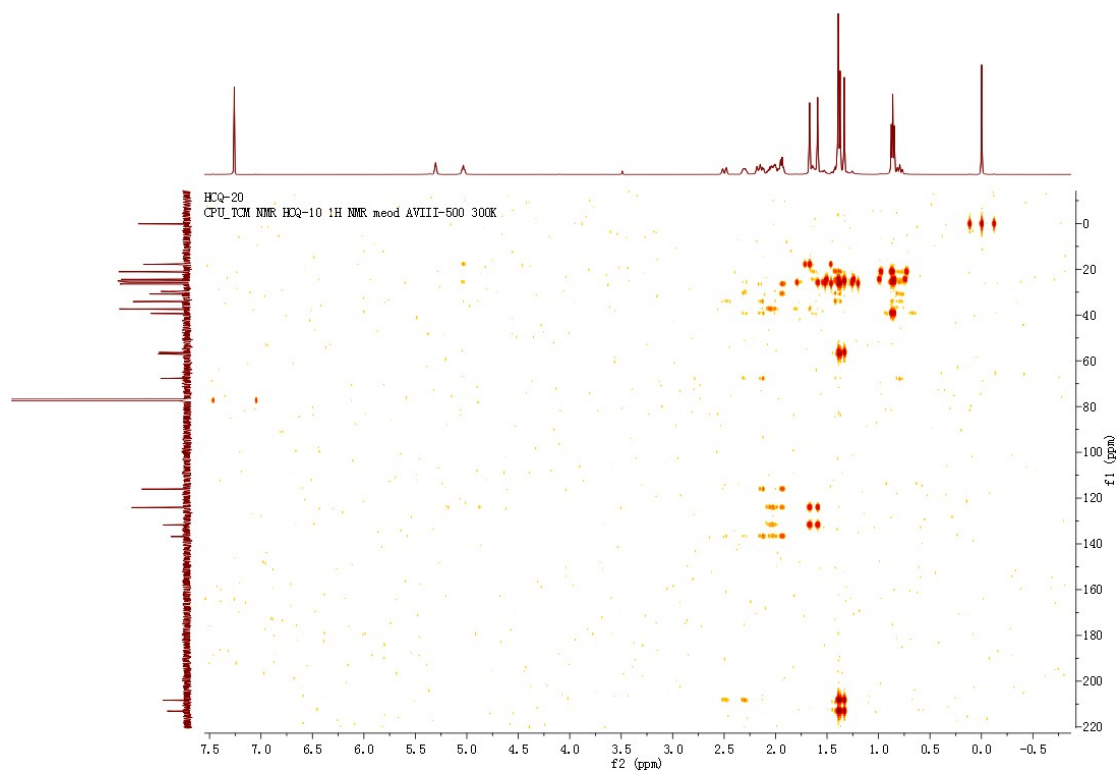


Figure S3.4 HMBC spectrum of compound **3** in CDCl_3

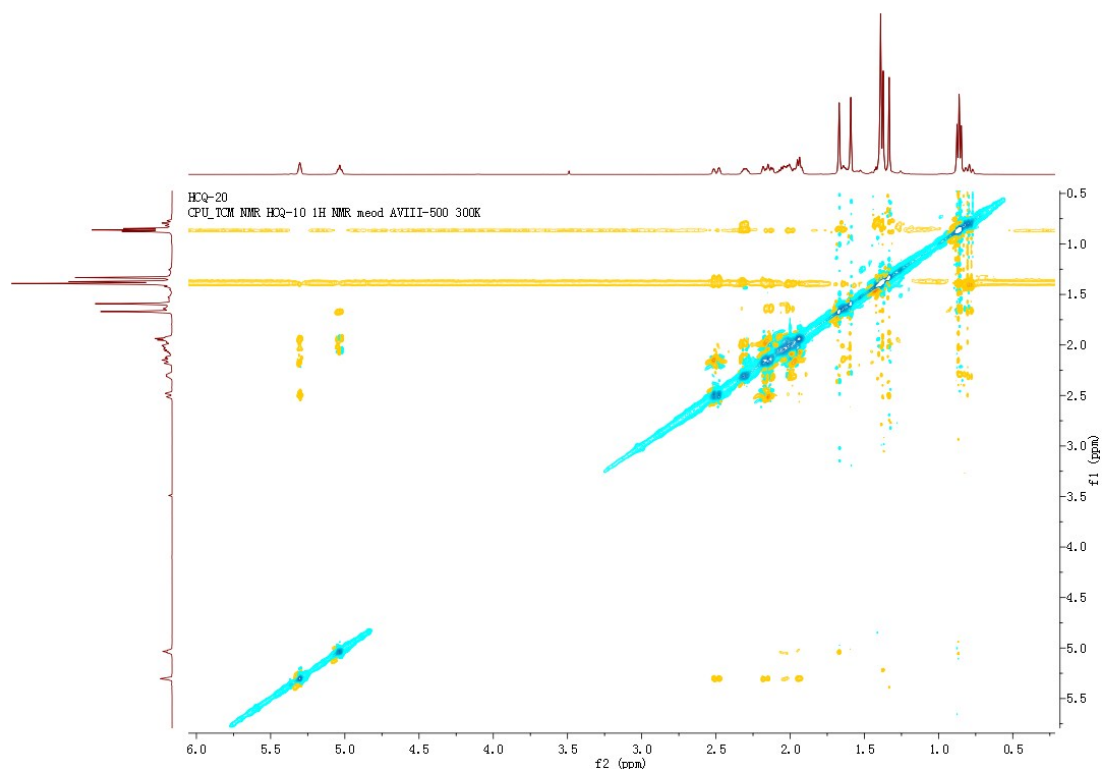
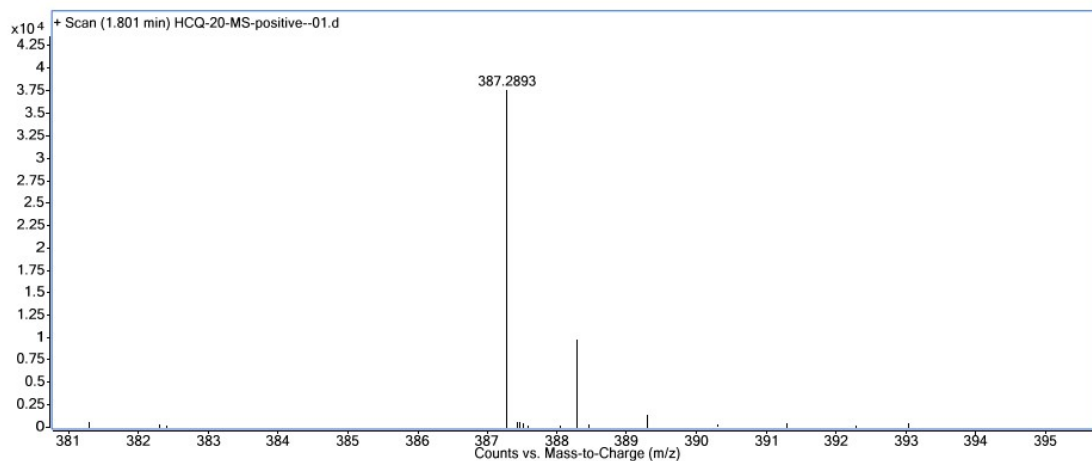


Figure S3.5 ROESY spectrum of compound **3** in CDCl_3



Elemental Composition Calculator

Target m/z:	387.2893	Result type:	Positive ions	Species:	$[\text{M}+\text{H}]^+$
Elements:	C (0-80); H (0-120); O (0-30); N(0-10); Na (0-5)				
Ion Formula	Calculated m/z		PPM Error		
$\text{C}_{25}\text{H}_{39}\text{O}_3$	387.2894		0.11		

Figure S3.6 HRESIMS spectrum of compound **3**

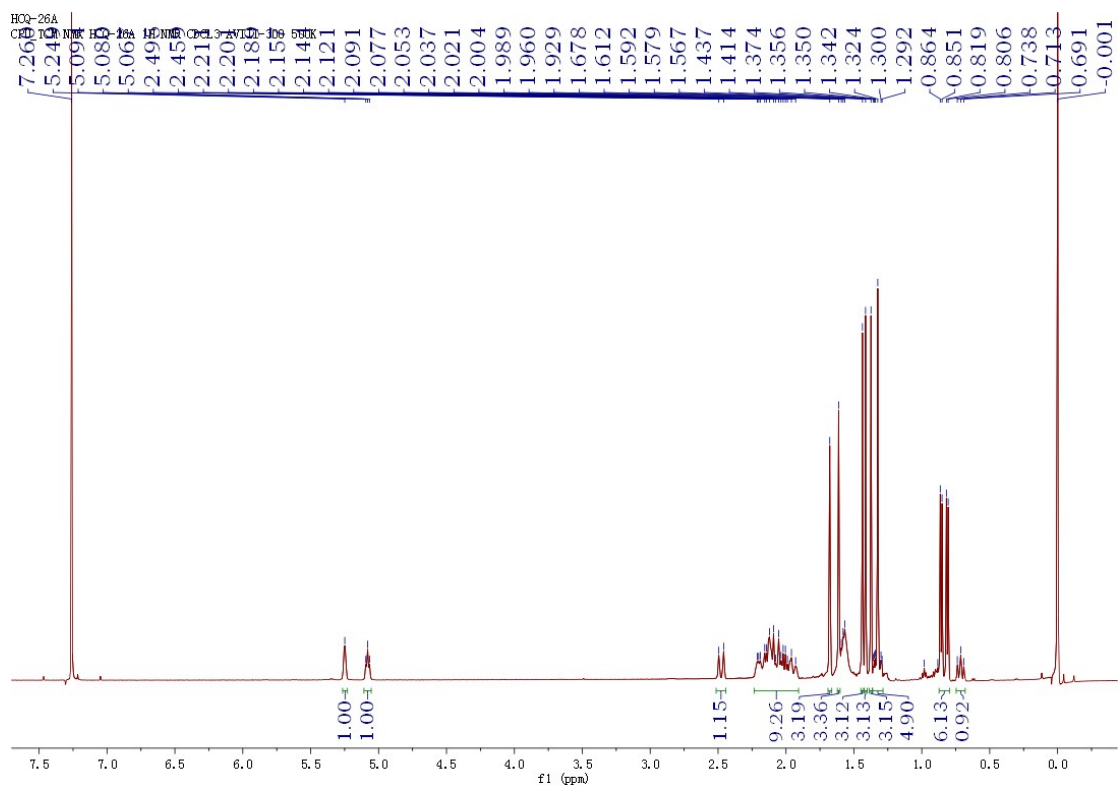


Figure S4.1 ¹H NMR spectrum of compound **4** in CDCl₃

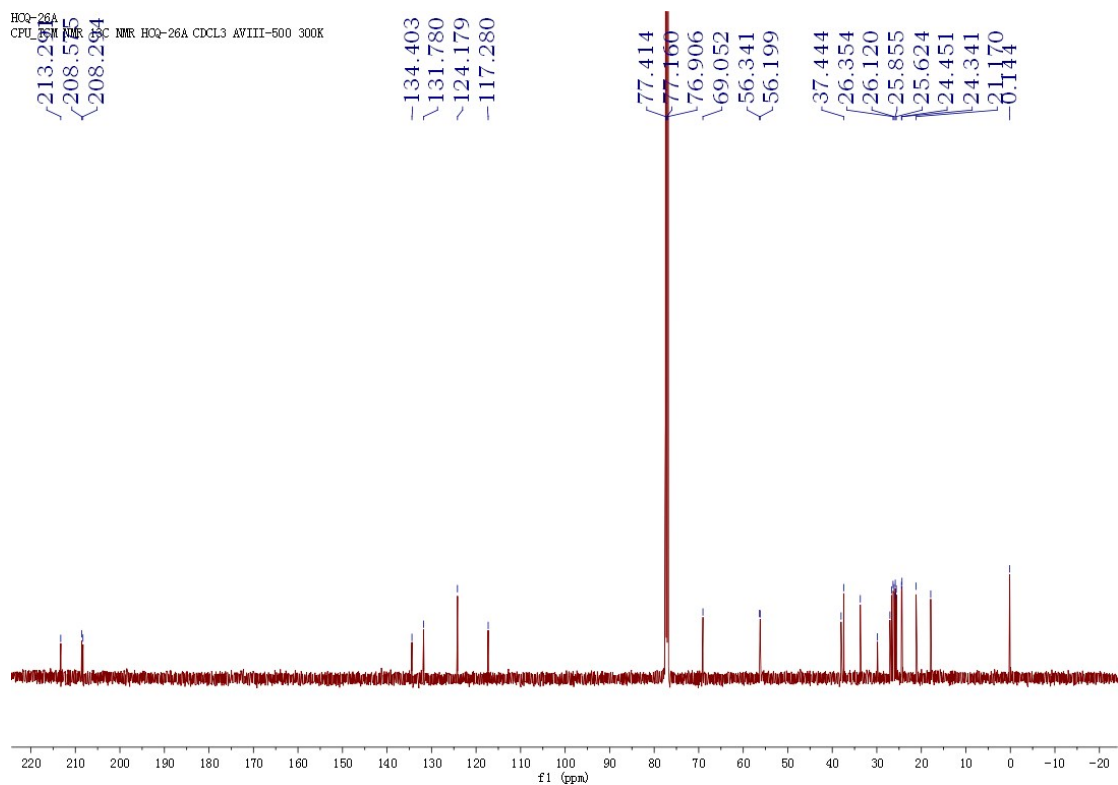


Figure S4.2 ¹³C NMR spectrum of compound **4** in CDCl₃

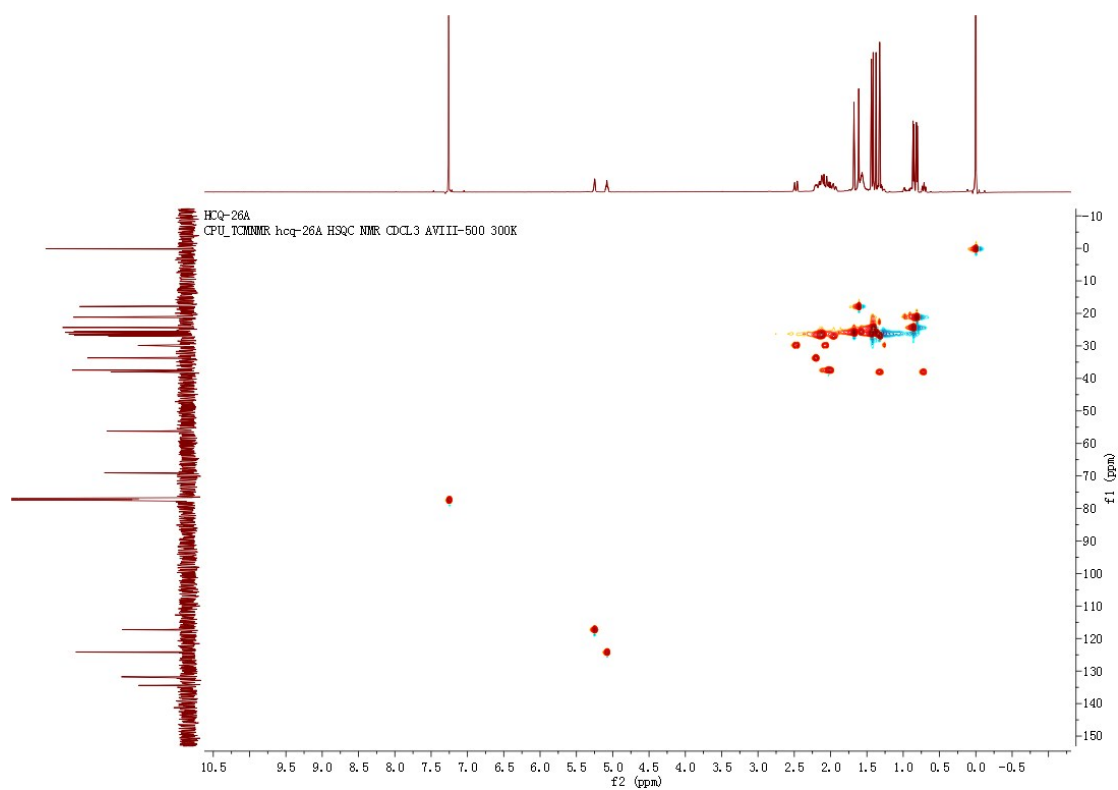


Figure S4.3 HSQC spectrum of compound **4** in CDCl_3

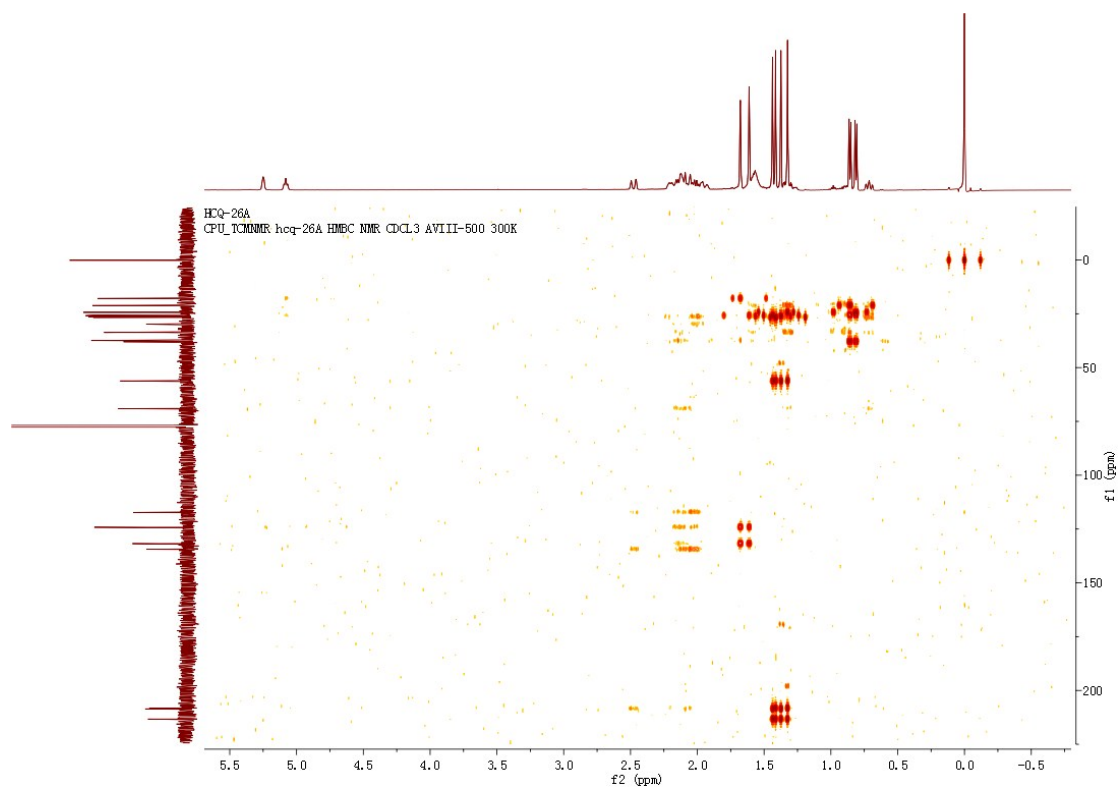


Figure S4.4 HMBC spectrum of compound **4** in CDCl_3

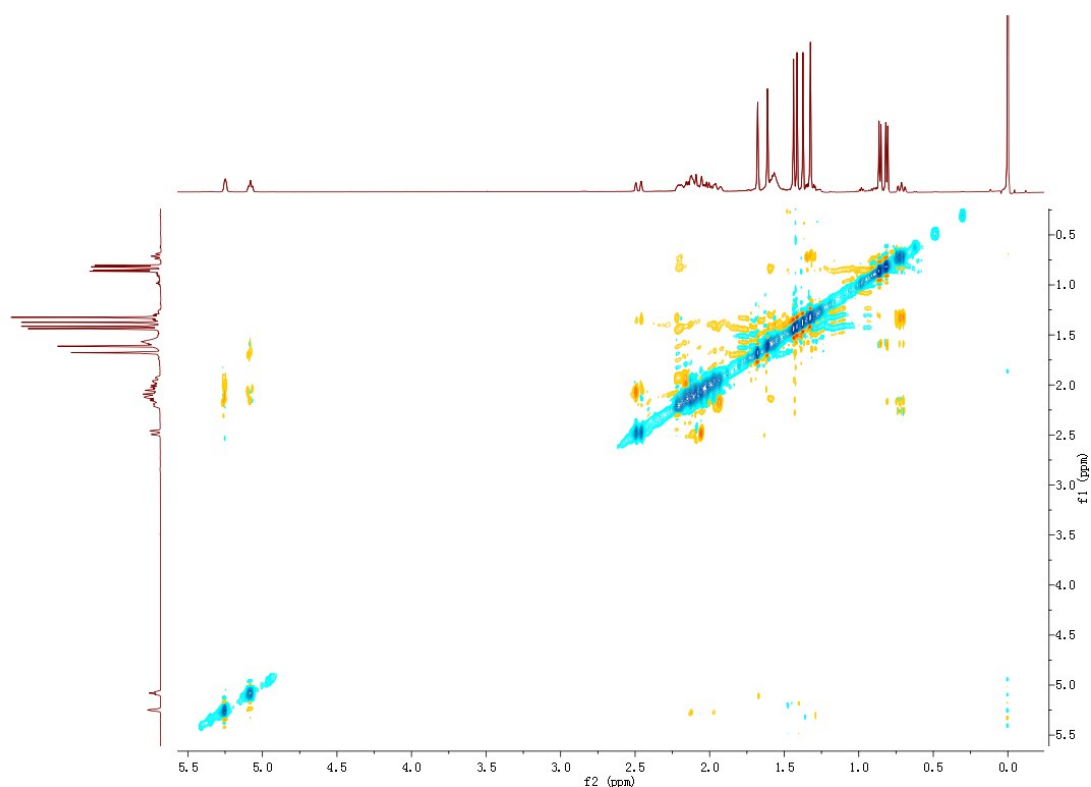
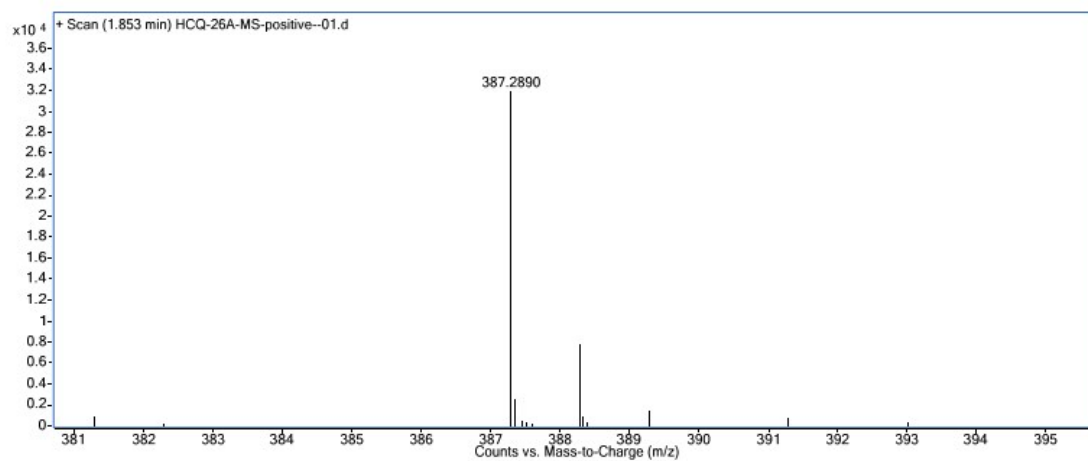


Figure S4.5 ROESY spectrum of compound **4** in CDCl_3



Elemental Composition Calculator

Target m/z:	387.289	Result type:	Positive ions	Species:	$[\text{M}+\text{H}]^+$
Elements:	C (0-80); H (0-120); O (0-30); N(0-10); Na (0-5)				
Ion Formula	Calculated m/z		PPM Error		
$\text{C}_{25}\text{H}_{39}\text{O}_3$	387.2894		0.9		

Figure S4.6 HRESIMS spectrum of compound **4**

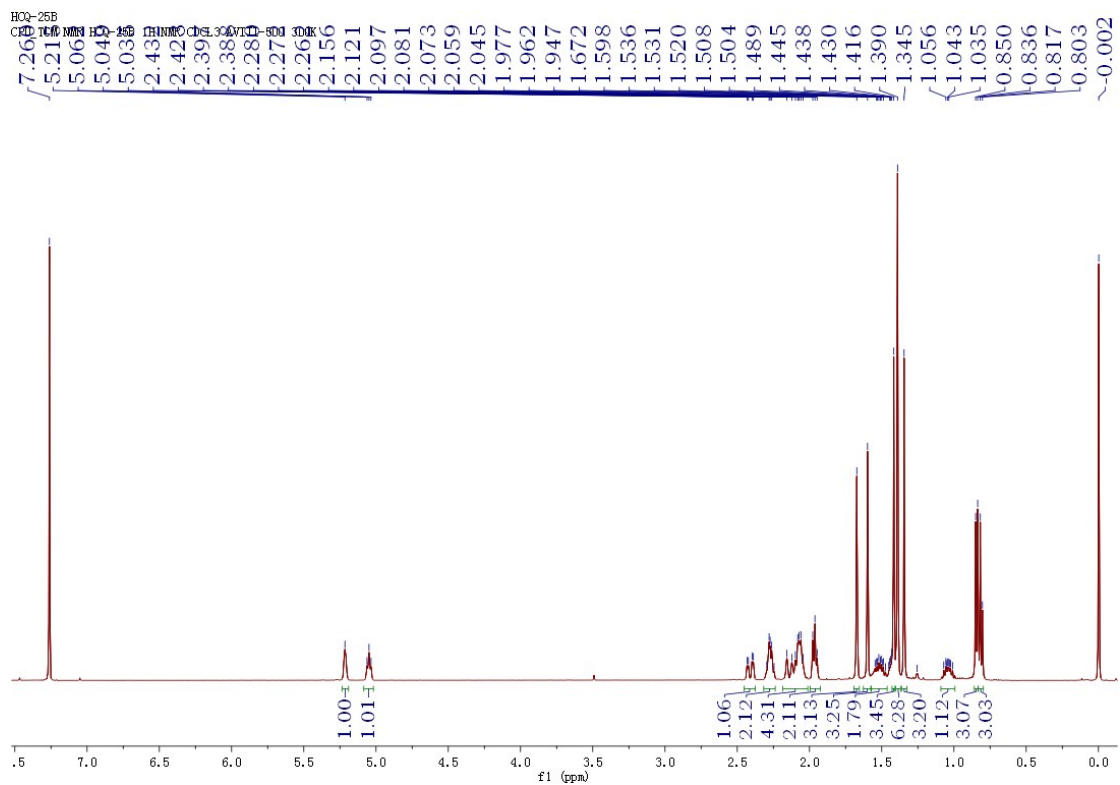


Figure S5.1 ^1H NMR spectrum of compound **5** in CDCl_3

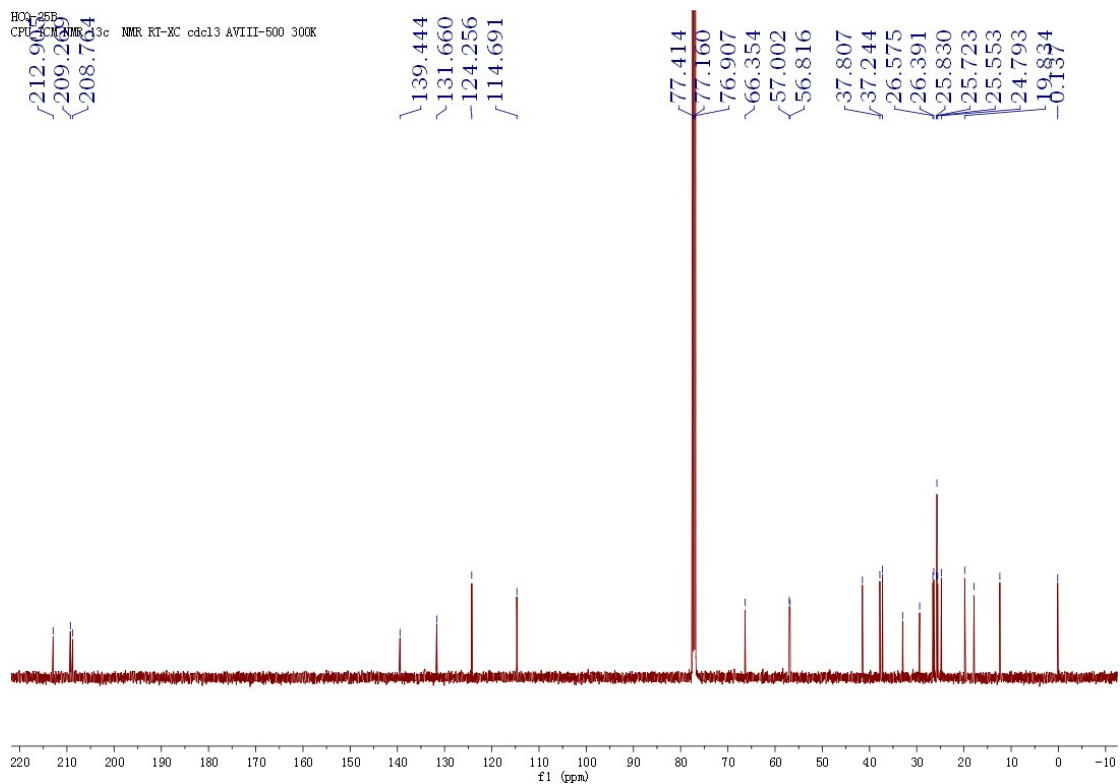


Figure S5.2 ^{13}C NMR spectrum of compound **5** in CDCl_3

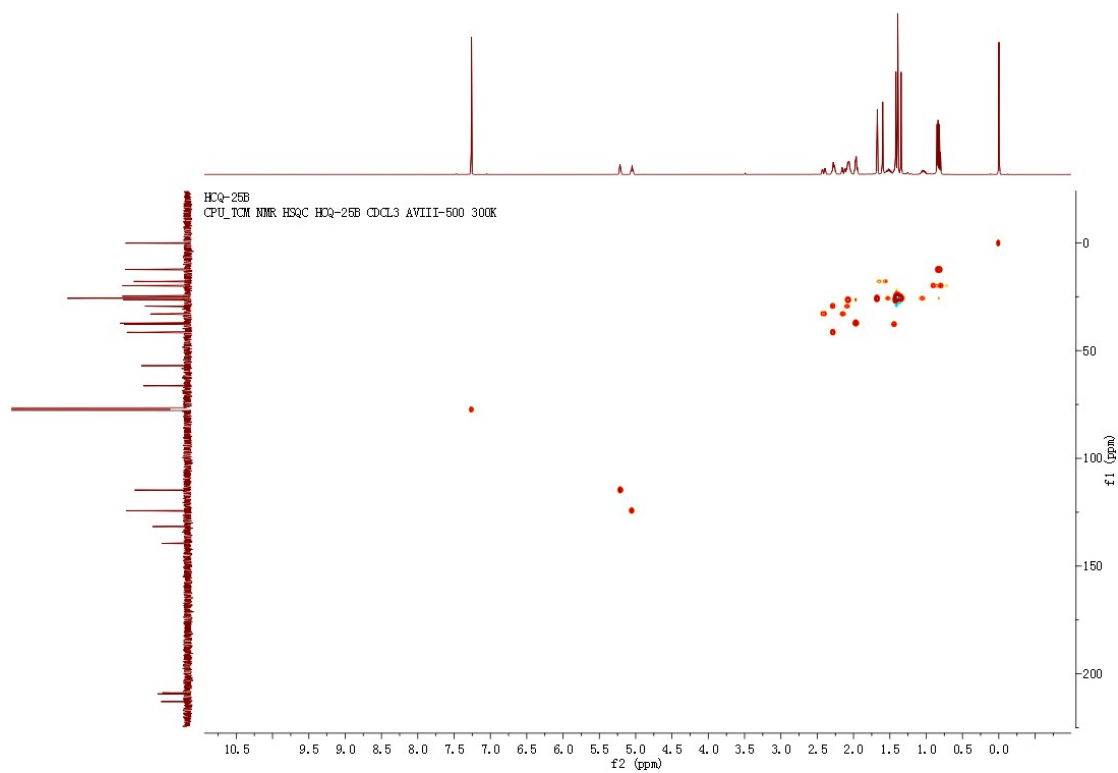


Figure S5.3 HSQC spectrum of compound **5** in CDCl₃

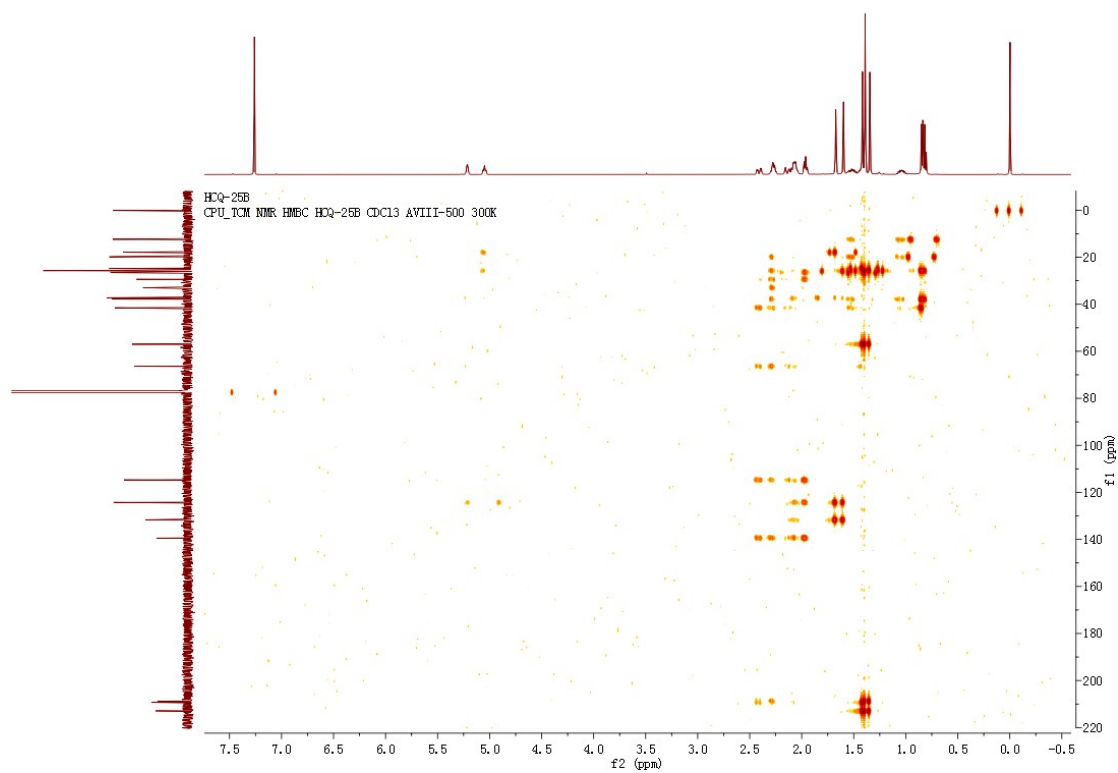


Figure S5.4 HMBC spectrum of compound **5** in CDCl₃

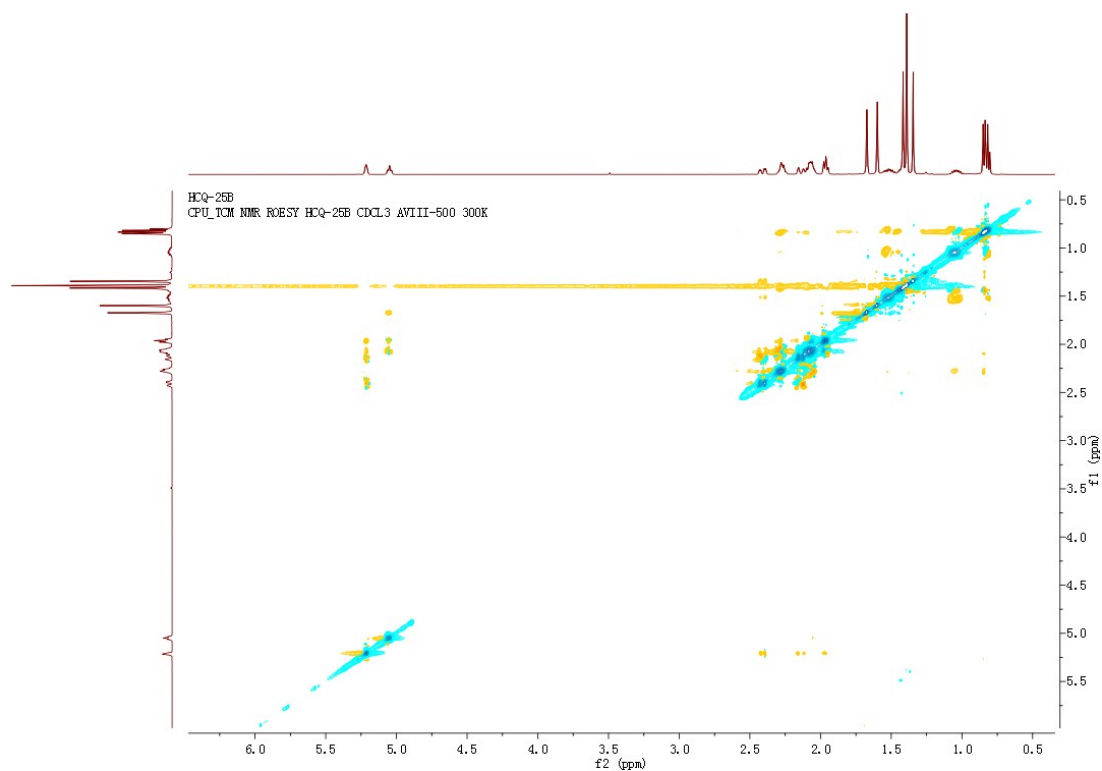
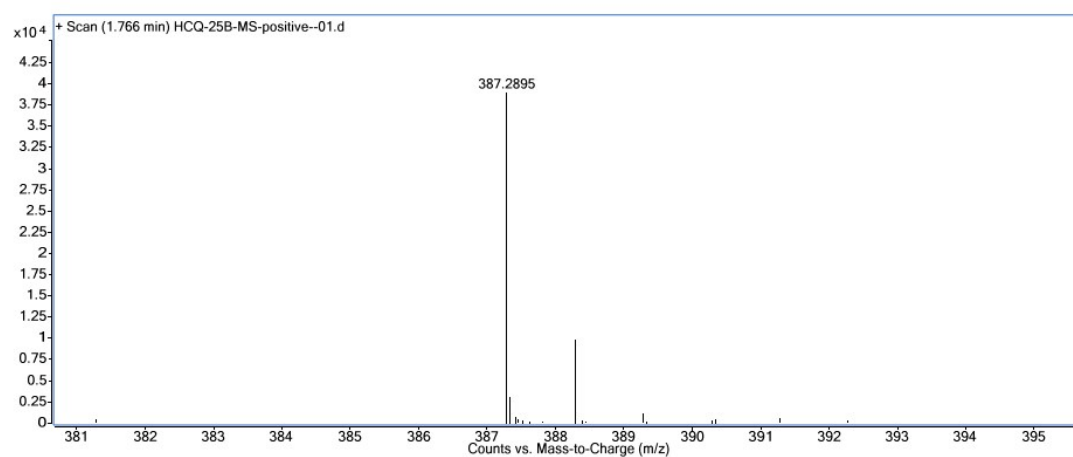


Figure S5.5 ROESY spectrum of compound **5** in CDCl₃



Elemental Composition Calculator

Target m/z:	387.2895	Result type:	Positive ions	Species:	[M+H] ⁺
Elements:	C (0-80); H (0-120); O (0-30); N(0-10); Na (0-5)				
Ion Formula	Calculated m/z		PPM Error		
C ₂₅ H ₃₉ O ₃	387.2894		-0.23		

Figure S5.6 HRESIMS spectrum of compound **5**

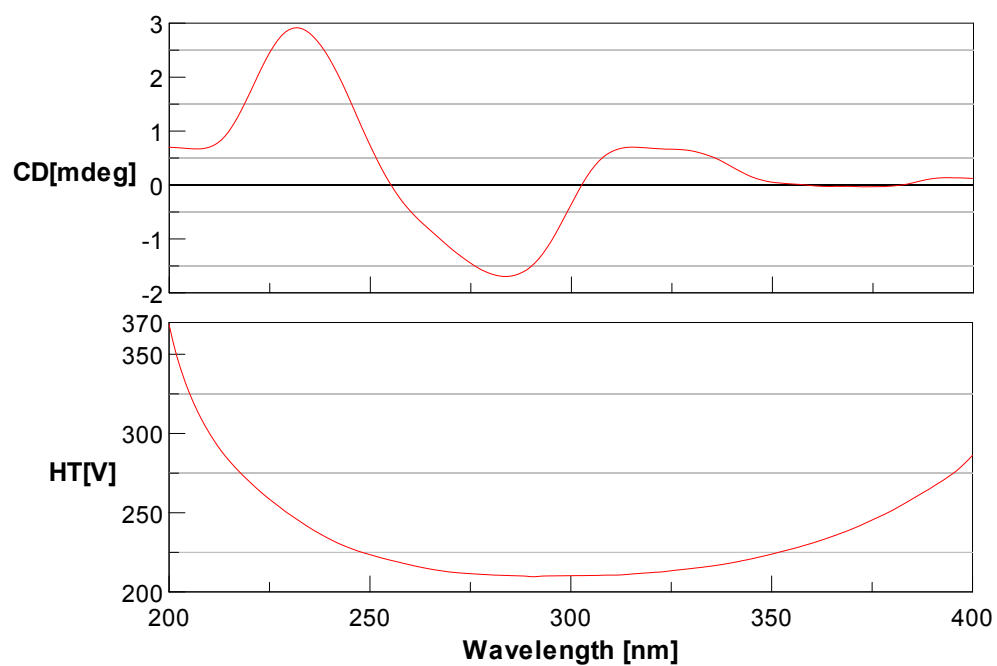


Figure S5.7 CD spectrum of compound **5**

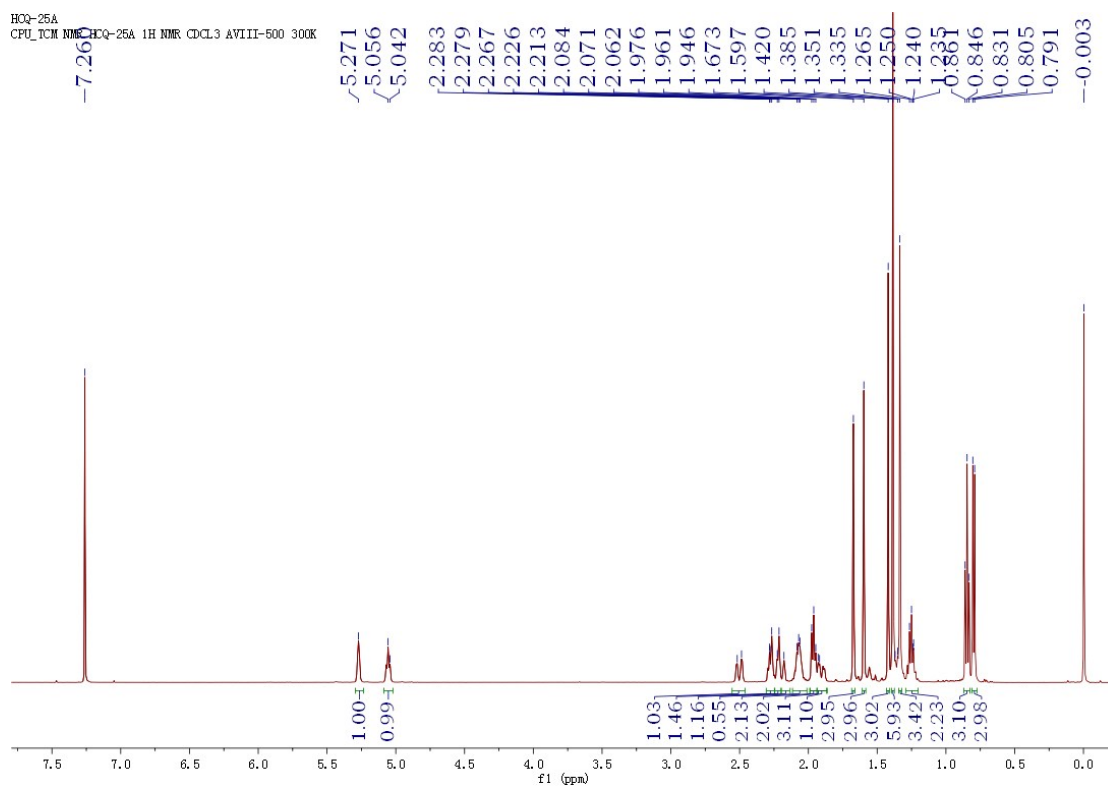


Figure S6.1 ^1H NMR spectrum of compound **6** in CDCl_3

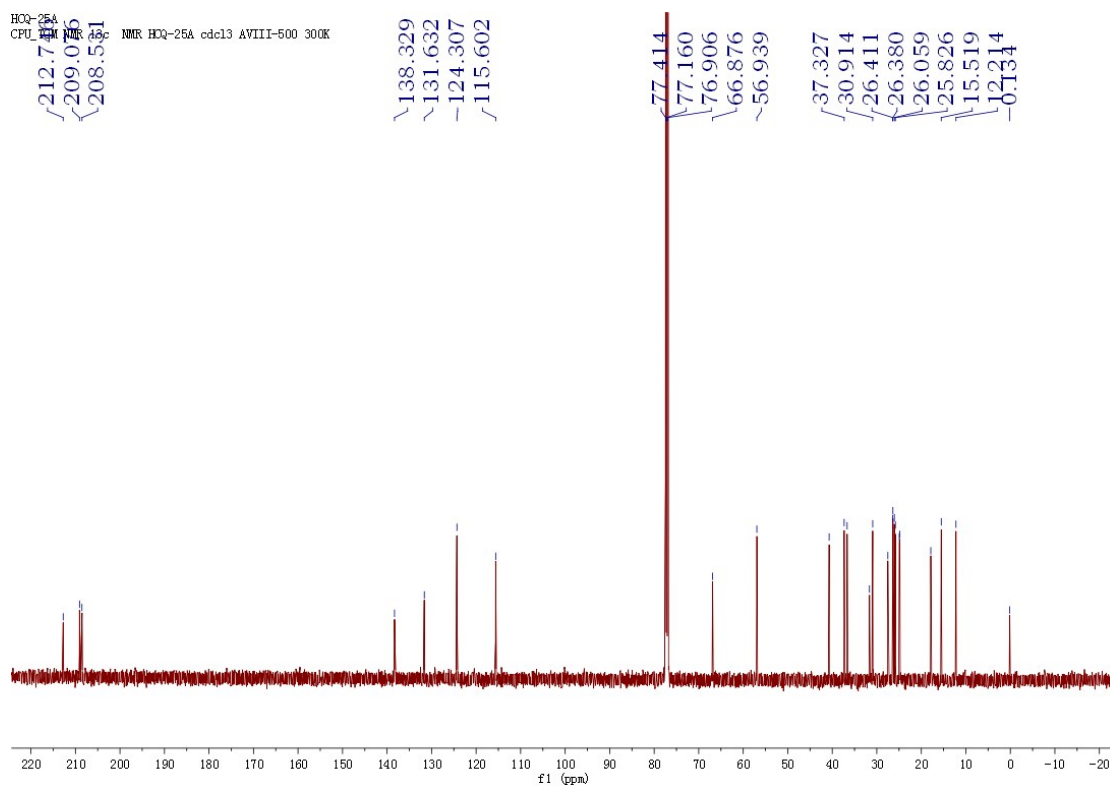


Figure S6.2 ^{13}C NMR spectrum of compound **6** in CDCl_3

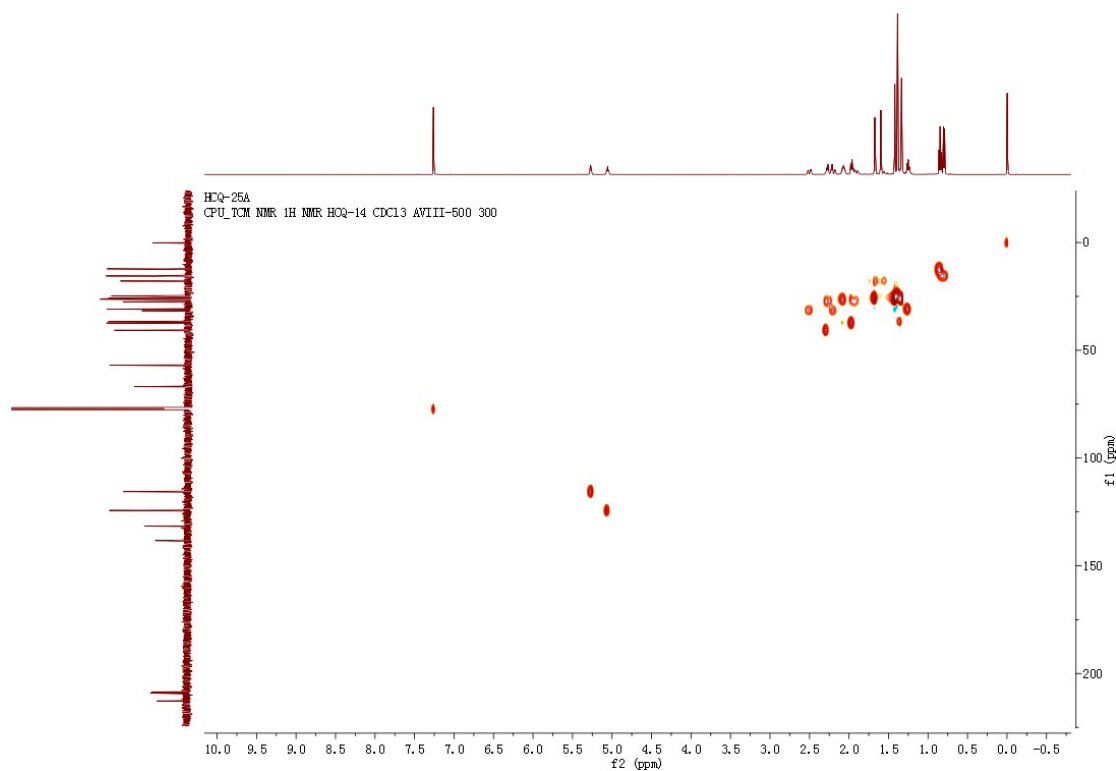


Figure S6.3 HSQC spectrum of compound **6** in CDCl_3

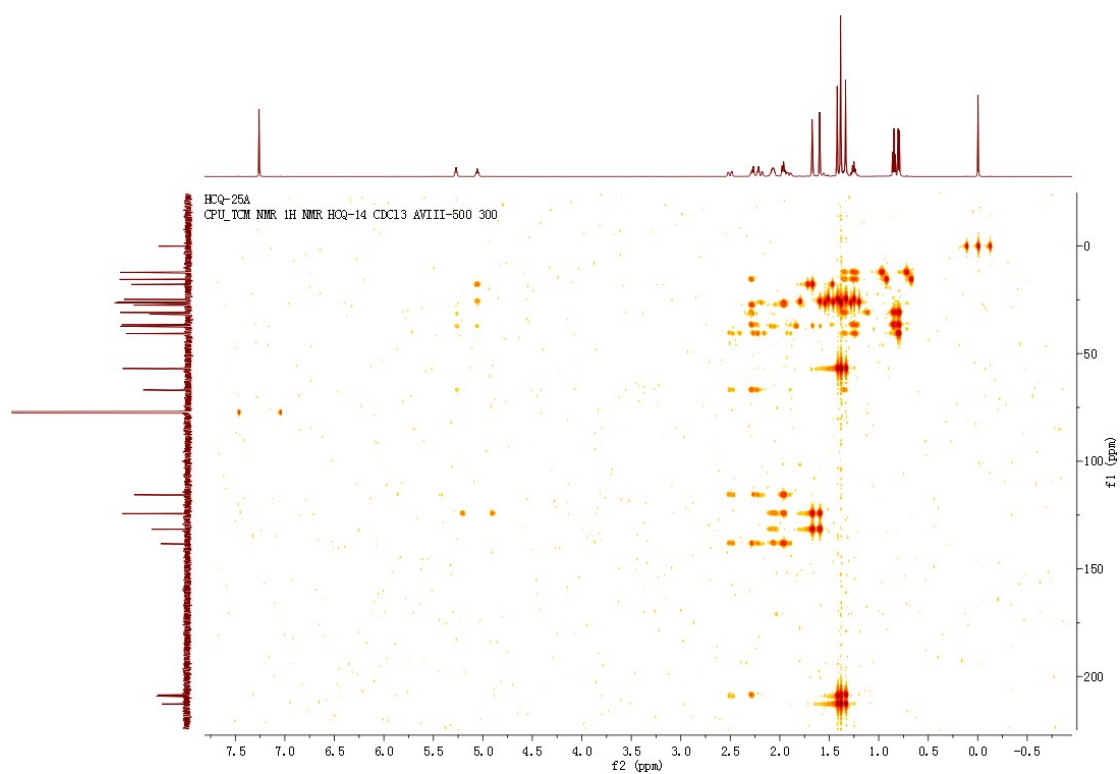


Figure S6.4 HMBC spectrum of compound **6** in CDCl_3

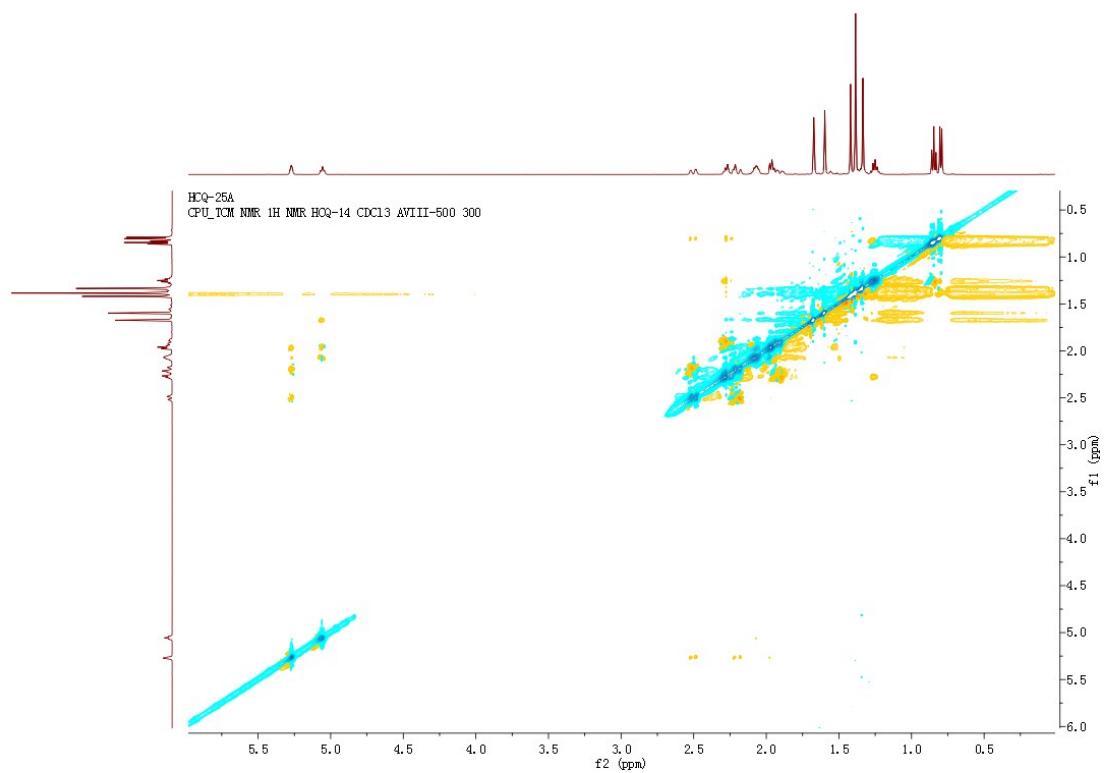
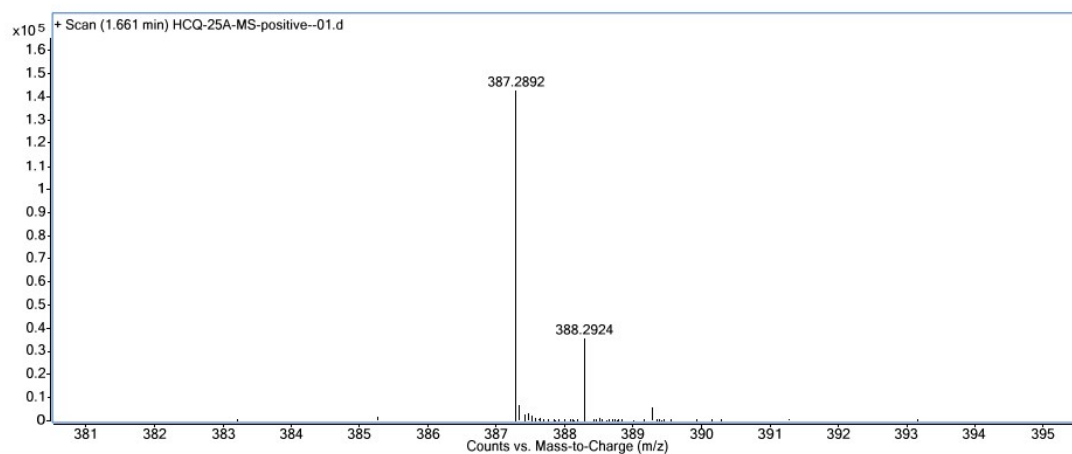


Figure S6.5 ROESY spectrum of compound **6** in CDCl_3



Elemental Composition Calculator

Target m/z:	387.2892	Result type:	Positive ions	Species:	[M+H] ⁺
Elements:	C (0-80); H (0-120); O (0-30); N(0-10); Na (0-5)				
Ion Formula	Calculated m/z		PPM Error		
C ₂₅ H ₃₉ O ₃	387.2894		0.43		

Figure S6.6 HRESIMS spectrum of compound **6**

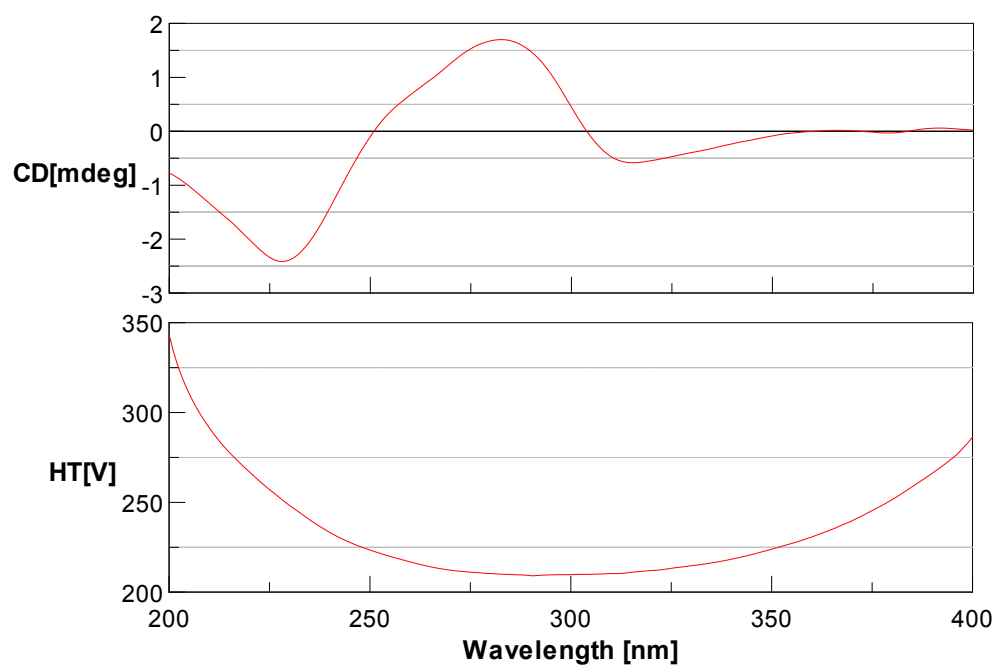


Figure S6.7 CD spectrum of compound **6**